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An Analysis Study of the impact of the main operating parameters on the ozone mass transfer rate in a Kenics Static Mixer Using the Steady State Back Flow Cell Model (BFCM)

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Abstract

The kenics static mixer (KMS) has been profoundly used in water and wastewater treatment processes, essentially in water ozonation for oxidation and disinfection purposes. since higher concentration of ozone is required, new contactors which operate efficiently at low gas/liquid ratio has been developed. The Kenics static mixer can fulfil these demands which lead to increase in the ozone mass transfer rate [1]. The main purpose of this paper is to use the steady state back flow cell model (BFCM) developed by Tizaoui and Zhang [1] so as to estimate the concentration profile of ozone in the liquid and the gas phases along the KMS. The study also aim to develop a Matlab code for the BFCM of the static mixer. Moreover, this research studied the effect of the main operating parameters: volumetric liquid mass transfer coefficient$(k_L a)$,the length of the Kenics static mixer, flow rate of water (L), and gas flow rate (G), back flow ratio $(B)$and the temperature on ozone concentration profile in the gas and liquid phases (y/y_{in}) and (x/x_{in}^*) respectively along the height of the Kenics static mixer.

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***Keywords*:** ozone mass transfer, back flow cell model, Kenics static mixer.

1. Introduction

A lot of processes in the field of chemical engineering are based on the chemical reaction between the solute gas and soluble species present in liquid. In nature, gas diffuses into the liquid through gas–liquid interface due to the concentration difference of the gas between the liquid at the surface and the liquid bulk without mechanical energy. But, the gas mass transfer rate is low and the reaction rate is also low. Therefore, gas-liquid contactors such as static mixers are used to obtain a higher gas mass transfer rate and correspondingly faster reaction. These contactors enhance the mass transfer rate by increasing surface area between the gas and liquid and increasing the intensity of turbulence [3, 4].

Ozonation is currently used as an alternative disinfection method to the chlorination process in water treatment, it has many drawbacks: it is incompatible with membrane processes and it result in formation of a dangerous organochlorinated compounds [5]. In water and wastewater treatment, ozone is used as biocide, oxidant and as pre-treatment reagent so as to improve the efficiency of the settling and filtration processes. Ozone is currently widely used because of it is ability to kill bacteria, viruses, spores and protozoa. The new stringent standards for drinking water require optimization of the ozonation process through improving the ozone gas mass transfer to the liquid phase [5, 6, 7]. The ozonation process is practised by dissolving gaseous ozone into the liquid water so as to react with target contaminants. Water ozonation is usually consists of four steps: convection and back mixing of the liquid flowing through contacting chambers inside the static mixer. These two processes occur simultaneously with two other processes: ozone gas mass transfer from gas phase to the liquid phase, ozone decomposition and reactions of ozone with organic material in the water [8].

The ozonation process is an effective method for removing the organic contaminants from water. It does not only depend on the mass transfer of ozone from the gas phase to liquid water, but also on the kinetic reactions of the ozone with the pollutants. The ozone mass transfer efficiency depends on the hydrodynamics of the fluids. However, the decay rate of the ozone depends on pH and temperature [9]. During the last few decades, new cheap ozone generators have been developed and they produce high ozone concentration, but they require low gas flow rates which result in low gas to liquid volumetric flow rate ratio. As a result, classical bubble columns are

no longer applicable because they require a larger gas flow rate to achieve efficient mixing between gas and liquid and therefore high ozone mass transfer. Static mixers, however, are more efficient at low gas/liquid ratio and high concentration of ozone and therefore they provide a solution to this problem. Moreover, static mixers produce a homogeneous ozone concentration because of the high turbulence produced by the elements that are inside the mixer, which ensure adequate gas/liquid mixing [1, 2].

Packed towers are extensively used for gas-liquid processes in many industries because of their effectiveness and cost. However, in the last few decades, static mixers have received a great attention because of their characteristics: high void fraction leading to low pressure drop with a very efficient gas-liquid contact and distribution [4] Since it is difficult to ensure adequate contact between the gas ozone and the liquid water in conventional bubble columns, static mixers have been developed as an attractive alternative in order to enhance the ozone mass transfer rate.

A static mixer, as shown in figure1, is designed as a series of identical, motionless inserts which are called elements. Its function is to redistribute fluid in a direction transverse to the main flow and in radial and tangential directions [4, 1].

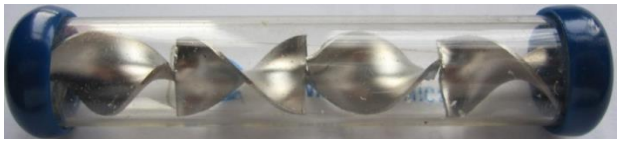

Fig. 1. Kenics static mixer (source: Chemineer Inc.[13])

Static mixers have many advantages over other gas-liquid contactors which can be summarised as follows:

- Small bubble diameter and therefore very high interfacial area
- High mass transfer coefficient
- Plug flow
- Little maintenance and low power consumption since they have no moving parts except the pump
- Higher performance at low energy consumption
- Narrow residence time distribution
- Low equipment cost
- Most of the factors mentioned above mean higher mixing between the ozone gas and the water enhanced heat and mass transfer [11, 12, 13]

Heyouni et al., (2002) [3] stated that the performance of a static mixer is better than other conventional gas-liquid contactors such as bubble columns and stirred vessels. This has been represented by figure 2.

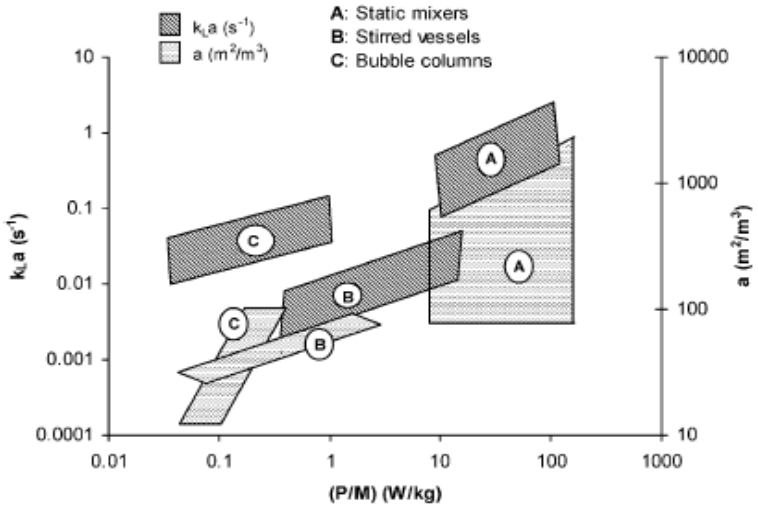

Fig. 2. Comparison of mass transfer coefficient and interfacial area between static mixers and traditional gas-liquid contactors [3].

Almost all the mathematical models that are developed to predict the performance of the ozone contactors are based on one of the following two assumptions: complete mixed flow or plug flow exist in the liquid phase. Applying these assumptions in modelling the gas-liquid contactors will underestimate the performance of the ozone contactor. Because of phenomena of the axial dispersion of the liquid phase, the real flow regime is closer to mixed flow than the plug flow, but it is not perfectly mixed flow. Thus, the back flow cell model (BFCM) has been developed as an alternative way to describe the hydrodynamics and mass transfer of the ozone inside the Kenics static mixer [10].

The BFCM is a general form of stagewise backmixing models and it can be used to characterise the backmixing in the liquid phase for co-current or counter-current gas-liquid contactors at steady state or unsteady state operating conditions [13].

The BFCM is a mathematical model that is applied to characterise the performance of the Kenics ozone static mixer. In order to describe the axial dispersion in the liquid phase, the BFCM assumes a back flow between the cells in the opposite direction to the main liquid flow and exchange flow in the same direction of the main liquid flow. These two flows have been

expressed as back flow ratio (B) and exchange flow ratio (B) and both of them are assumed to be equal and constant along the mixer. Generally, BFCM is composed of two series of equal number of completely mixed cells in which one series describes the liquid phase and the other describes the gas phase. It uses the cells number and back flow ratio to describe the backmixing in the liquid phase [13].

Gamal El-Din and Smith (2001a) [5, 11] have developed a transient BFCM as alternative approach to the axial dispersion model and continuous flow stirred tanks in series in order to describe the hydrodynamics and the back mixing in the liquid phase in the ozone bubble contactor.The result of their model is shown in figure 3.

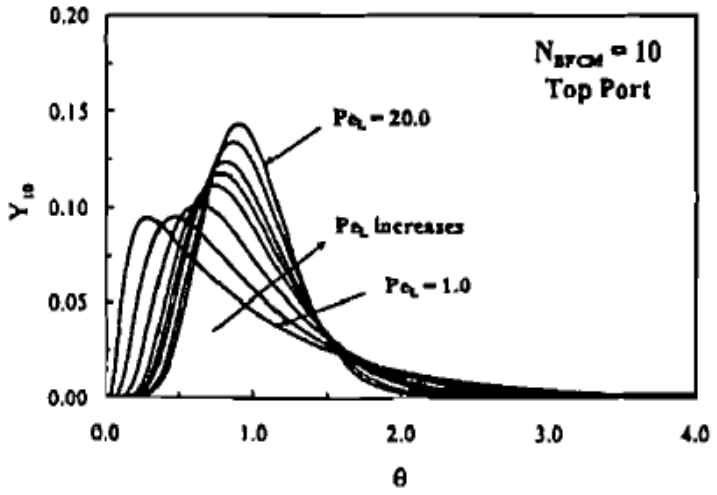

Fig. 3. Theoretical RTD curves for different Peclet numbers (Gamal El-Din and Smith (2001a)[11])

Baawain et al (2007) [7] have modified the steady state BFCM in order to account for variable mass transfer coefficient along the height of the impinging-jet bubble column. The data from their model is shown in figure 4.

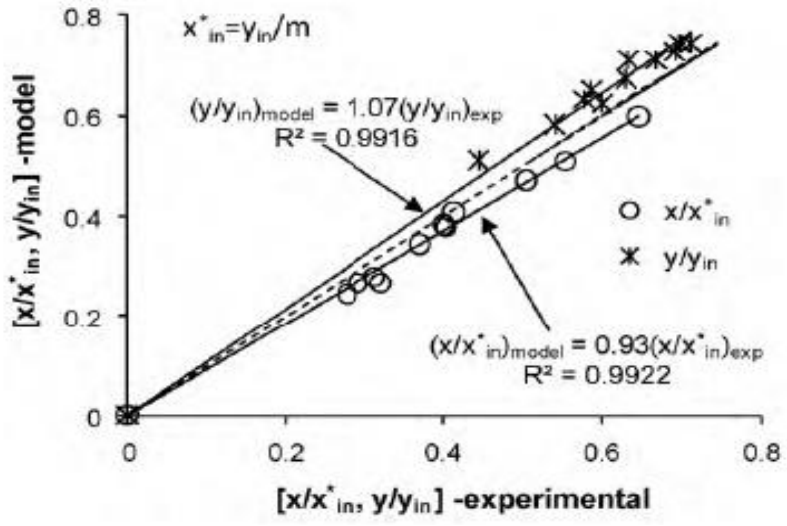

Fig. 4. The relation between model and experimental outcome [7]

The steady state BFCM has been developed by performing a basic material balance with respect to the ozone was performed around each cell inside the static mixer. The ozone mass transfer rate of ozone to the water and also its reaction in the main bulk of the liquid phase were included in the basic mass balance equations.this paper aims to use the steady state back flow cell model (BFCM) developed by Tizaoui and Zhang [1] to determine the concentration profile of ozone in the liquid and the gas phases along the KMS. Moreover, a Matlab code for the BFCM of the static mixer has been developed. Furthermore, the effect of the main operating parameters was discussed: volumetric liquid mass transfer coefficient($k_L a$) ,the length of the Kenics static mixer, flow rate of water (L), and gas flow rate (G), back flow ratio (B) and the temperature on ozone concentration profile in the gas and liquid phases (y/y_{in}) and (x/x_{in}^*) respectively along the height of the Kenics static mixer.

2. Results and Discussion

The BFCM of Tizaoui and Zhang [1] has been built to predict the ozone concentration profile in a Kenics static mixer. Figure 5 below shows a schematic representation of BFCM for upward co-current flow conditions in the static mixer.

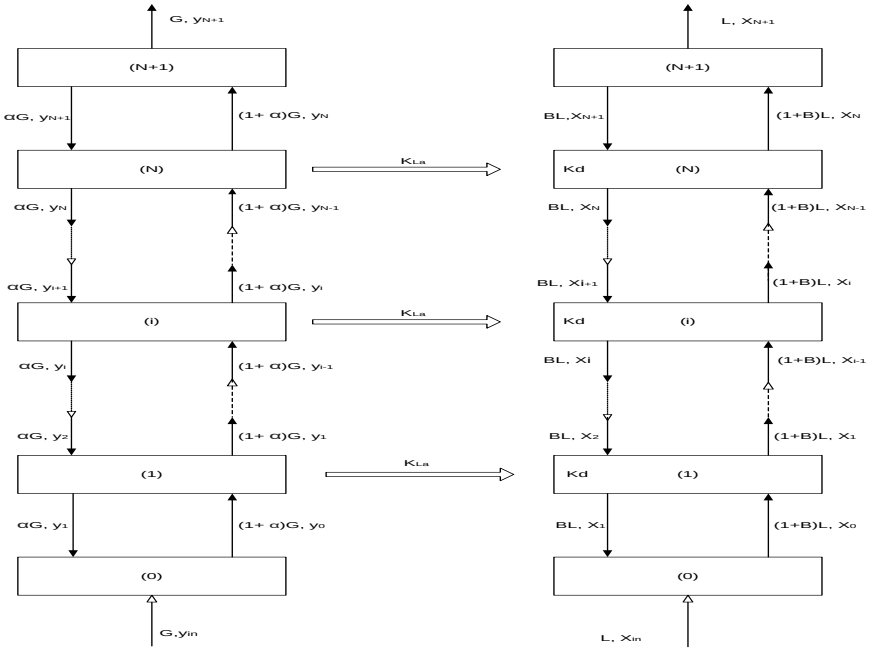

Fig. 5. Schematic representation of the steady state BFCM

The ozone mass transfer rate (Ψ) can be estimated according to the two-film theory model:

$\Psi = k_L a\ (x_L^* - x_L)$ (1)

Where: Ψ is the ozone mass transfer rate per unit volume, $k_L$is local liquid mass transfer coefficient, $a$is specific interfacial area, x_L^* is the concentration of dissolved gas in equilibrium with bulk gas and x_L is the concentration of the dissolved gas in the bulk liquid.

The $k_L a$ value used in this study is 0.1 s^{-1} [3].

The equilibrium liquid concentration of ozone x_i^* can be calculated by the following formula:

$$x_i^* = y_i / m \quad (2)$$

$$m = \frac{H}{P_T} \quad (3)$$

Where: P_T is the total pressure drop across the static mixer and H is the Henry's constant and it is estimated by the following formula [4]:

$H = 3.84 \times 10^7 (10^{pH-14})^{0.035} exp(-2428/T)$ (4)

Hoigne (1982) (cited in Gamal El-Din and Smith [5]) mentioned that as gaseous ozone dissolves in the liquid water and due to its very high oxidative nature, it begins to decay by auto-decomposition and oxidation of pollutant present in water. The ozone decay rate or the ozone chemical reaction ratedepends on water temperature, pH and water content and it can be described by the following correlation [6]:

$R = Ek_dC_i$ (5)

$k_d = 5.43 \times 10^3 \exp(-4964/T)$ (6)

Where k_d is the pseudo first order auto decomposition rate constant in (s^{-1}), where its value is equal to 2.4030e-004S^{-1} and the T is the temperature in K[1,5].

Hatta number is used to account for the contribution of the chemical reaction to the mass transfer process:

$$Ha^2 = \frac{D_{O_3} k_d}{k_L^2} \quad (7)$$

The value of the ozone diffusivity coefficient D_{O_3} is equal to 1.76 × 10^{-9} m^2/s [2].

From equation7, it was found that the value of the Hatta number, Ha =6.5033e-006.

For upward and co-current mode shown in Figure 1, the basic mass balance for the ozone dissolved in the gas phase in each cell is:

For i = 0: $Gy_{in} + \alpha Gy_1 - (1+\alpha)Gy_0 = 0$ (8)

For 1 ≤ i ≤ N:

$$(1+\alpha)Gy_{i-1} + \alpha Gy_{i+1} - \alpha Gy_i - (1+\alpha)Gy_i - k_l a v_c (x_i^* - x_i) = 0 \quad (9)$$

For i=N+1$(1+\alpha)Gy_N - \alpha Gy_{N+1} - Gy_{N+1} = 0$ (10) Now, the mass balance of the dissolved ozone in the liquid phase:

For i = 0: $Lx_{in} + BLx_1 - (1+B)Lx_0 = 0$ (11)

For i =1:

$$(1+B)Lx_0 + BLx_2 - (1+B)Lx_1 - BLx_1 + k_l a v_c (x_1^* - x_1) - k_d x_1 = 0 \quad (12)$$

For 2 ≤ i≥ N:

$$(1+B)Lx_{i-1} + BLx_{i+1} - (1+B)Lx_i - BLx_i + k_l a v_c (x_i^* - x_i) - k_d x_i = 0 \quad (13)$$

For i = N: $(1+B)Lx_N - BLx_{N+1} - Lx_{N+1} = 0$ (14)

The equations above have been summrised and numerically solved by Matlab 2014. (See Appendix)

2.1. The concentration profile along the height of the static mixer

Figure 6: presents the liquid and gas concentration profile of the ozone along the height of the Kenics static mixer. The characteristics of the Modelled static mixer are: 39 cells inserted in line through the length of the mixer, total length of 0.74m, internal diameter of 0.0191m and it operates at gas to liquid volumetric ratio of 0.22. The gas and liquid flow rates and inlet ozone concentration values are 0.41L/min, 1.8L/min and 64g/m^3 respectively.

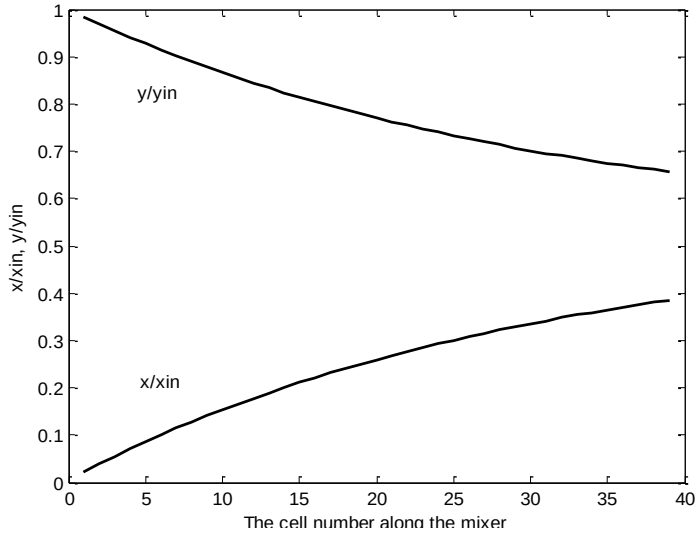

Fig. 6. The ozone concentration in the gas and liquid phase along the height of the static

From the graph, it can be clearly seen, and as was expected that the ozone concentration in the gas phase (y/y_{in}) decreases across the height of the static mixer. On the other hand, the ozone concentration in the liquid phase (x/x_{in}^*)increases as the liquid passes along the height of the static mixer. This trend in the ozone concentration profile can be explained by the fact that the main purpose of the water ozonation process inside the Kenics static mixer is to transfer the ozone from the gas phase to the liquid phase so the ozone can reacts with pollutants present in the water. The exit ozone concentration in the gas phase and the liquid phase are still far from the equilibrium state which can be defined as the state at which the ozone gas concentration (y/y_{in}) is equal to the ozone liquid concentration (x/x_{in}^*).

This non-equilibrium state ($y/y_{in} \neq x/x_{in}^{*}$) is due to the short contact time between the gas phase and the liquid phase inside the static mixer [1].
There is a slightly more rapid decrease in the ozone gas concentration and also more rapid increase in the ozone liquid concentration at the bottom of the Kenics static mixer. This may be because of the higher degree of turbulence and higher shear rates at the entrance of the mixer which results in smaller bubbles and therefore larger gas-liquid interfacial area and subsequently higher mass transfer rate of ozone from the gas phase to the liquid phase [9].

2.2. The effect of the volumetric mass transfer coefficient ($K_L a$) on the ozone mass transfer

The volumetric liquid mass transfer coefficient is key parameter to describe the rate of ozone mass transfer in a Kenics static mixer. It is the product of the interfacial area (a) and liquid mass transfer coefficient (k_L). The impact of physical variables such as density, surface tension and viscosity and the process variables such as flow rates of gas and liquid and the mixer shape and dimension can be represented by the $k_L a$ [1]. Since the Ozone gas is slightlysoluble in water, the resistance to ozone mass transfer in the gas phase is assumed to be negligible. Consequently, the liquid film is the controlling factor for the ozone mass transfer rate. In this model, the rate of ozone mass transfer in the Kenics static mixer was estimated by the following kinetic correlation (eq.1):

$$\Psi = K_L a V \Delta C$$

The model was run to simulate the change in the gas and the liquid concentration profile along the column as a function of the volumetric mass transfer coefficient ($K_L a$) so that the approach to equilibrium can be studied. As shown in figure 7, and as the $K_L a$ increased from $0.09s^{-1}$ to $0.2s^{-1}$, a continuous increase in the dissolved ozone concentration in the liquid phase occurred along the mixer whereas continuous reduction in the dissolved ozone concentration in the gas phase occurred along the mixer and also at the outlet of the static mixer. For all values of $K_L a$ and especially at the highest value of $0.2s^{-1}$, most of the gaseous ozone was consumed before reaching the top of the mixer height and this leads to a lower driving force for the mass transfer process and therefore results in a smaller amount of ozone residual in the effluent stream. At larger $K_L a$ values, the increasing and the decreasing trends in the ozone concentration profile in the liquid and gas phase respectively were faster than those at low $K_L a$. This is due to the

high value of the mass transfer rates that cause faster depletion of the ozone in the gas phase and faster transportation of ozone to the liquid phase. It is very noticeable from the graph that the liquid ozone concentration (x/x_{in}^{*}) at K_La =0.2s^{-1} has dramatically increased from around 0.06 at the first cell to about 0.5 at cell number 25 and after that it slightly and steadily increased along the rest of the mixer height. However, at K_La =0.09s^{-1}, the ozone liquid concentration has monotonically increased along the height of the mixer. Based on these observations, it has been concluded that a smaller number of cells are required for the high values of K_La.

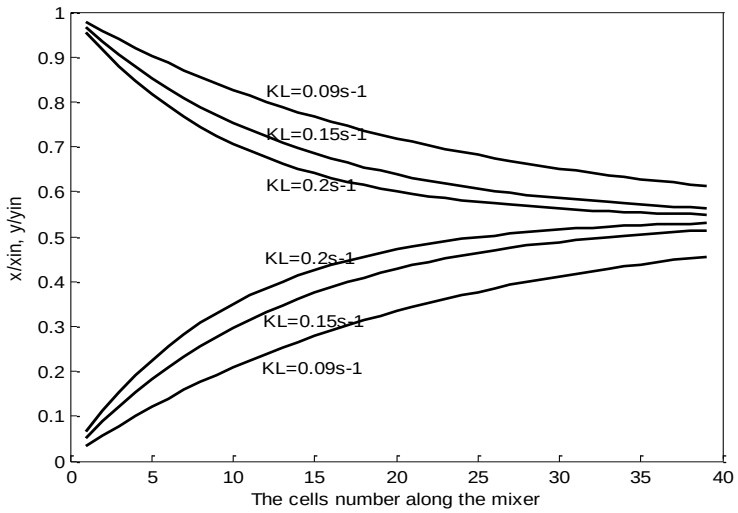

Fig. 7. The effect (k_La) on the performance of the KSM

2.3. The effect of the length of the Kenics static mixer (L) on the ozone mass transfer

Figure 8 illustrates the impact of the length of the Kenics static mixer on the gas and liquid concentration profile of the ozone along the height of the static mixer. The performance of the mixer has been tested at three different lengths: 0.74, 2, 2.8m.

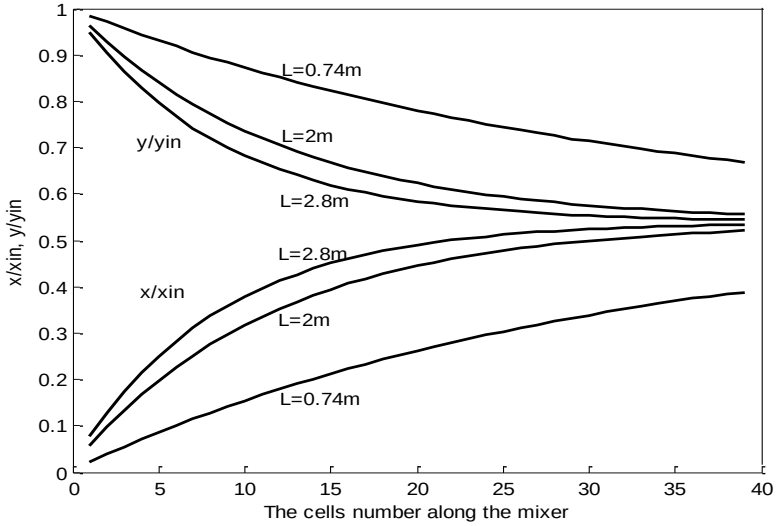

Fig. 8. The effect of the height on the performance of the SM

As it can be seen from the figure 8, and as the length of the mixer increases, there has been a continuous decrease and increase in the gas and liquid concentration of the ozone respectively along the height of the mixer and also at the outlet of the contactor. The static mixer of 2.8m length has provided the best performance in terms of approaching the equilibrium between the gas and liquid ozone concentration. In theory, the equilibrium state between gas and liquid can only be reached by using a static mixer of an infinite length [1]. A static mixer of 2m length has achieved relatively similar results to the 2.8m length static mixer and therefore it can be considered as the optimum choice because the gas and liquid concentrations of the ozone are closer to equilibrium than the 0.74m length mixer and at the same time it has less capital cost than the 2.8m length mixer.

2.4. The effect of the gas and liquid flow rates (G and L) on the ozone mass transfer

Figures 9 and 10 depict the effect of gas and liquid flow rates on the gas and liquid concentration profile of the ozone.

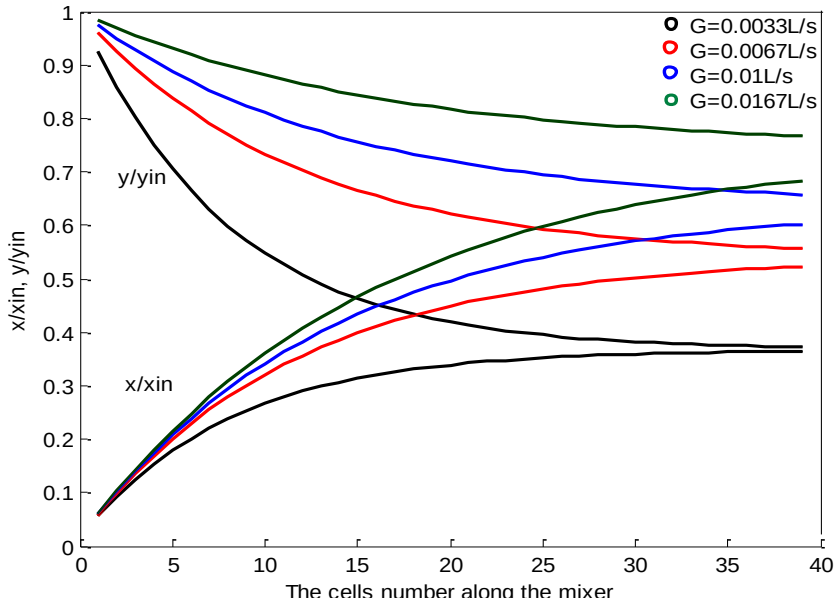

Fig. 9. Effect of the gas velocity on the ozone concentration

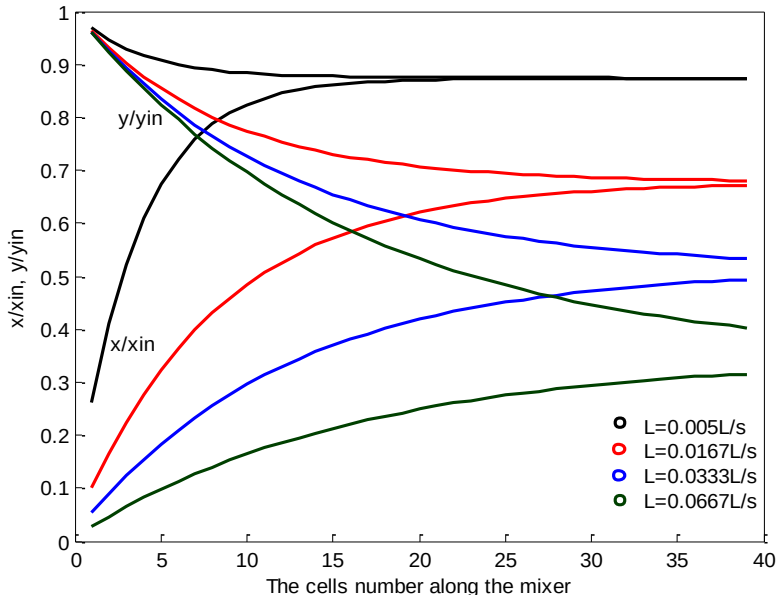

Fig. 10. The effect of liquid velocity on the ozone concentration

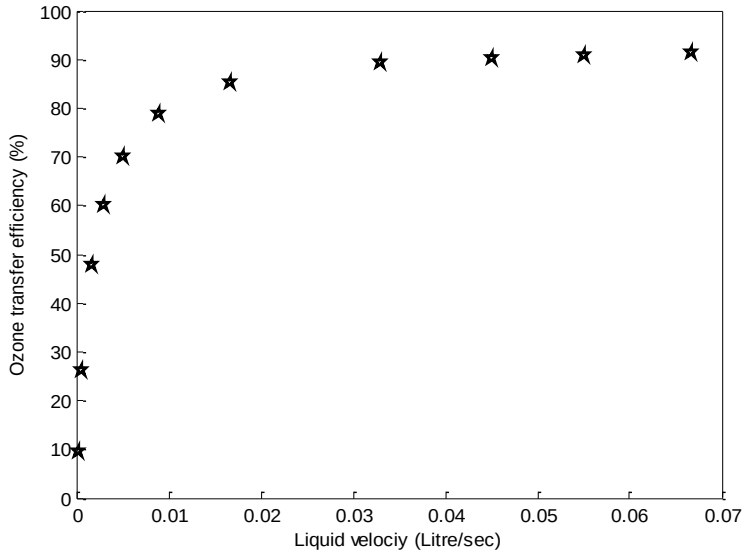

Fig. 11. The relation between the liquid velocity and the ozone mass transfer efficiency of the mixer

In figure 9, and as the gas flow rate was increased from 0.0033L/s to 0.0167L/s at a given liquid flow rate, the exit ozone liquid concentration (x/x_{in}^{*}) increased from around 0.3 to 0.7 and the exit ozone gas concentration (y/y_{in}) decreased from about 0.8 to 0.4. On the other hand, as shown in figure 10, increasing the liquid velocity from 0.005 L/s to 0.0667L/s results in a decrease in the liquid concentration (x/x_{in}^{*}) from 0.87 to 0.25 and also the gas concentration has dropped from 0.9 to 0.3. Based on these observations, it can be said that increasing the gas flow rate resulted in an increase in the rate of mass transfer of ozone from the gas phase to the liquid phase whereas increasing the liquid flow rate leads to a reduction in the rate of ozone mass transfer. This can be ascribed to the fact that increasing the gas velocity will lead to a smaller gas-liquid interfacial area and therefore higher volumetric mass transfer coefficient, but increasing the liquid velocity results in a larger interfacial area. These results agree with the findings of Sanchez et al., [10] and also with the findings of Heyouni et al., [3]. They stated that the higher the value of the gas velocity, the larger the diameter of the gas bubbles. However, the bubble diameter decreases as the liquid velocity increase. This has been ascribed to the fact that higher energy input is required for high liquid velocities. This high power results in higher turbulence which causes the large bubbles to break into smaller bubbles. Thus, it results in higher ozone mass transfer

efficiency. However, when Heyouni et al., [3] studied the effect of gas and liquid velocities on the interfacial area(a) and the mass transfer coefficient ($k_L a$), It was found that the ($k_L a$) and (a) increase with increasing the either the gas or liquid velocities.

Gamal El-Din and Smith [11] have mentioned that the back flow ratio increases with increasing the gas flow rate. This can be explained by the fact that as the gas flow rate increases, the sizes of the bubbles increase with increasing the gas flow rate leading to a higher degree of circulation inside the mixer and therefore high backmixing. On the other hand, the back flow ratiodecreases as the liquid flow rate increases. This is because the liquid flow approaches the plug flow regime at higher liquid flow rates.

Ozone transfer efficiency is a key design parameter due to the fact that most of the energy used in the water ozonation process is consumed in the ozone generation stage. Therefore, the loss of ozone in the off-gas can cause the process to be uneconomical [1].

$$\text{Ozone transfer efficincy} = \frac{y_{i,N} - y_{yi,0}}{y_{i,N}} \times 100 \qquad (15)$$

As shown in figure 11, as the liquid velocities increased from 0.001 to 0.05L/s, the ozone transfer efficiency increased from 10 to 93%. However, increasing the liquid flow rate to values above 0.05L/s resulted in very little improvement in the ozone transfer efficiency. The ozone transfer efficiency reaches maximum values at the highest liquid flow rates but with low G/L ratio. These results confirm the findings of the experiment of Craik et al., [12], where it was found that the maximum ozone mass transfer efficiency was obtained at high liquid velocity and low gas/liquid superficial velocity. These results prove the fact that the static mixers achieve the high ozone mass rates at low gas flow rate and low gas to liquid flow ratio (G/L).

2.5. The effect of the temperature on the ozone mass transfer

The effect of the temperature on the gas and liquid concentration at the outlet of the mixer was studied and the results are shown in figure 12. The figure shows that the exit gas concentration (y/y_{in}) is more sensitive to changes in temperature than the liquid concentration (x/x_{in}^{*}).

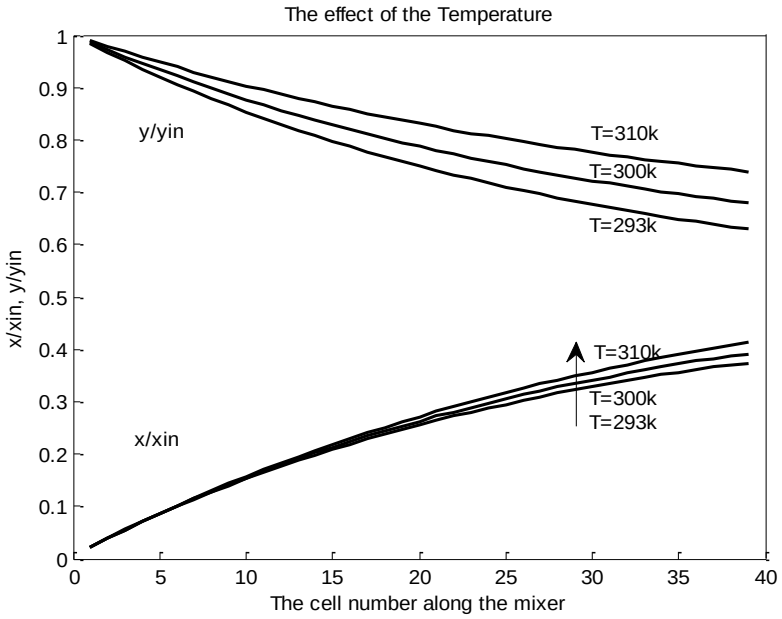

Fig. 12. The effect of the temperature on the ozone concentration

Figure 12 shows that as the temperature increases, the ozone liquid concentration at the outlet of the mixer increases while the exit gas concentration decreases. These observations can be compared to the theoretical understanding of the ozone reactions in the liquid phase. The slow chemical reaction occurs in the liquid bulk (water) after gas (ozone) absorption and it causes a reduction in the ozone concentration in liquid bulk and its rate is described by the following correlations (eq.5 and eq.6).

The temperature is inversely proportional to the first order rate constant of ozone decay (k_d) in water. Thus, high temperatures will result in smaller values of k_d and subsequently lower reaction rate and therefore the ozone concentration in the liquid phase will be larger than those concentrations at lower temperatures.

2.6. The effect of the back flow ratio (B) in the liquid phase on the ozone mass transfer

The back flow ratio (B) can be defined as the fraction of the inlet main liquid flow to each cell that returned back from the upper stage to the lower adjacent stage. The strong backmixing of the liquid phase which is prevalent in the static mixers is because of pumped fluid through the mixing elements is divided the fluid into several partial streams and then redistribute these streams in opposite direction to the main flow in order to form a combined

and homogeneous mixture. Back mixing is characterised by two parameters: number of stages and the Peclet number and is estimated by the following equation:$B = \frac{N_{BFCM}}{Pe_L} - 0.5$. In the steady state BFCM, a value of 0.33 has been assigned to the back flow ratio (B) as it has been reported in the study of Tizaoui and Zhang, [1].

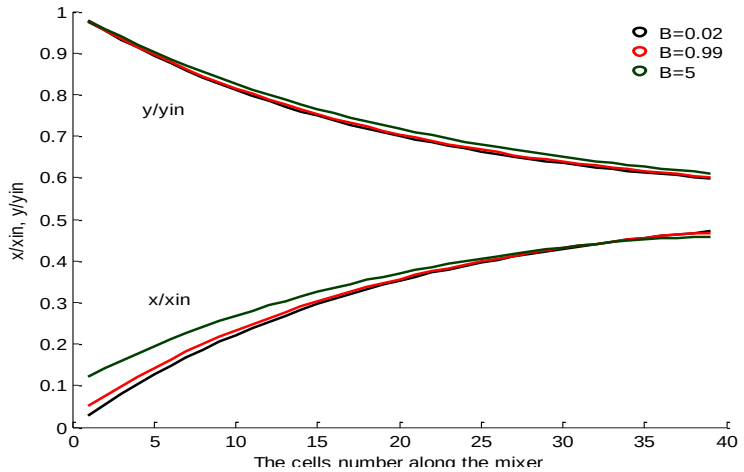

Fig. 13. The impact of the back flow ratio (B) on the ozone concentration profile

Figure 13 presents the effect of the back mixing in the liquid phase on the ozone gas and liquid concentrations along the static mixer. As the back flow ratio increases from 0.02 to 5, the liquid ozone concentration at the entrance of the static mixer (x/x_{in}^*) has increased from 0.03 to 0.12 while the ozone liquid concentration at the top of the static mixer remains almost the same.The ozone concentration in the gas phase (y/y_{in}) has a slightly increased along the whole height of the static mixer and this is maybe because of the backmixing in the gas phase was assumed to be negligible due to the high buoyancy of the gas phase. In contrast, the ozone concentration in the liquid phase (x/x_{in}^*) has only increased at the bottom of the mixer, but this increase in the concentration is becoming less noticeable as the liquid passes through the bottom of the static mixer. However, at the top of the static mixer, the liquid concentration has remained the same for all three values of B. This can be explained by the fact that the liquid flow approaches plug flow conditions as it flows toward the top of the static mixer. As a result, the degree of back mixing decreases to a negligible value at the top of the mixer and therefore there is no change in the liquid ozone concentration at the top of the static mixer. In a study conducted by Munter

[2], it was found that at B=500, the decolorization degree spasmodically increased from zero to around 78%.

3. Conclusion

The steady state BFCM has predicted the gas and liquid ozone concentration profile across the height of the Kenics static mixer. The equations of the model have been numerically solved and transformed into the form of matrices and then implemented in a Matlab software.

The impact of the main characteristic parameters of the steady state BFCM on ozone concentration profile in the gas and liquid phases along the height of the Kenics static mixer were analyzed using the Matlab software. These parameters are:

- The back flow ratio in the liquid phase
- The length of the Kenics static mixer
- Gas and liquid flow rates
- Volumetric liquid mass transfer coefficient
- Temperature

The effect of the liquid flow rate on the ozone concentration profile in the gas and the liquid phase and the ozone mass transfer efficiency of the mixer have been studied. It was found that the higher the liquid flow rates, the lower the ozone liquid concentration. Regarding the mass transfer efficiency, it was found that as the liquid flow rate increased it resulted in lower gas/liquid ratio, which increased the ozone mass transfer efficiency to around 94%. The later results proved the fact that the static mixers are more efficient at low gas/liquid ratio. Thus, static mixers can be successfully used for water ozonation.The backmixing ratio has relatively little impact on the ozone liquid concentration. However, this impact reduces to a negligible value as the liquid flows toward the top of the mixer. Moreover, better mass transfer efficiency was obtained at higher lengths of static mixer but this will also result in higher capital cost and therefore a trade off is required.

4. Further work

The steady state BFCM should be further developed and expanded in order account for the chemical reactions, especially the bromate formation.

The steady state BFCM should be further developed to account for the following parameters: (1)The backmixing in the gas phase should be considered in order to study its influence on the hydrodynamic performance

of the Kenics static mixer, especially in the cases where the gas phase largely deviates from the plug flow regimes; (2)Variable back flow ratio in the liquid phase along the height of the static mixer should be included in the model. Since there is larger degree of mixing taking place at the inlet of the mixer than the outlet of the mixer, variable back flow ratio should be included in developing the BFCM, especially for the tall static mixers; (3) Variable cell volume along the height of the static mixer should be considered in developing the model and this very useful when modelling static mixers with multiple cells of variable dimensions; (4) The models should be modified and expanded to account for variable mass transfer coefficient and cross sectional area along the Kenics static mixer.

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6. Appendices

Appendix I - The steady state back flow cell model

```
function[x,y,xs,u,s,d] = BFCM(N,V,L,G,T,PH,Pt,Kl,B,xin,yin)
D = 1.76*10^-9;
%D, ozone diffusivity coefficient
Kd = 5.43*10^3 * exp(-4964/T)
%Kd, pseudo first order ozone decay rate constant
Kl=0.1
%Kl, Volumetric liquid side mass transfer coefficient
Ha =sqrt((D*Kd)/Kl^2)
% Ha, Hatta number
if (Ha<1)
%D, ozone diffusivity coefficient
% Call Function[x,y,xs,u,s] =
BFCM(39,0.0054,0.03,0.0067,293.15,7,980,0.1,0.33,0,0.0640)
%INPUT
% N,cell number , % V, liquid cell volume
% L, liquid flow rate % G, Gas flow rate
% T, Temperature = 20 C = 293.15 K
% PH, acidty of water=7 ,% Pt, Total pressure = 2 atm
% Kl. volumetric liquid mass transfer coefficient= 0.1 s-1
% B, back flow ratio = 0.33
% xin, inlet ozone liquid mole fraction
% yin, inlet ozone gas mole fraction
% OUTPOT
% x,ozone mole fraction in the liquid through the column
% y, mole fraction of zone in the gas through the column
% xs, equilibrium liquid mole fraction
% u, ratio = y/yin
% s, ratio = x/xsin  where Xsin,is the inlet equilibrium mole fraction=yin/m
Kd = 5.43*10^3 * exp(-4964/T)
% Kd is the reaction rate constant
% d = 1.74*10^-9;
% Kw=4.667*10^-4;
% K=2*10^-3;
% Ha =sqrt((d*Kw)/K^2)
% if (Ha<1)
%Kd = 0.028
H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T)
% H is the henry constant
```

```
m = H/Pt
a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 = (Kl*V)/G;
LM = zeros(N,N);
LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) + diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;
LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);
GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);
GB = zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);
A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;
x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;
relrem = (y(N)-y(1))/y(N)
%relrem is ozone transfer percentage
u = y/yin;
xsin = yin/m;
s = x/xsin;
f=1:1:39
figure(1)
plot(f,u,'k',f,s,'r')
xlabel('the mixer length, z'), ylabel('x/xin, y/yin')
disp('      x       y       xs      u       s ');
disp([x,y,xs,u,s,[1:length(x)]'])
end
end
```

Appendix II - the effect of the main parameters of the steady state BFCM

```
clear all
close all
clc
for i=1:6
if i==1
for Kl=[ 0.09 0.15 0.2 0.3];
N = 39;V =0.00553;L = 0.03;G = 0.00667;T = 293.15;PH=3;Pt = 980;B = 0.33;xin = 0;yin
= 0.064;
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on
plot(f,u,'k',f,s,'r')
```

```
xlabel('The cell number'), ylabel('x/xin, y/yin'),title('The effect of  mass transfer
coefficient')
end
end
if i==2
for G=[0.0033 0.0067 0.0133 0.0167 ];
N = 39;V =0.0054;L = 0.03;T = 290;PH=6;Pt = 880;Kl= 0.1;B = 0.33;xin = 0;yin = 0.064,
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on,plot(f,u,'k',f,s,'r')
xlabel('The cell number'), ylabel('x/xin, y/yin'),title('The effect of gas flow rate')
end
end
if i==3
for B=[ 0.02 0.99 5]
N = 39;V =0.0054;L = 0.03;G = 0.00667;T = 293.15;PH=3;Pt = 880;Kl= 0.1;xin = 0;yin =
0.064
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on,plot(f,u,'k',f,s,'r')
xlabel('The cell number'), ylabel('x/xin, y/yin'),title('The effect of Backmixing ratio(B)')
end
end
if i==4
for V=[0.0054 0.0147  0.0206 ]
N = 39;L = 0.03;G = 0.00667;T = 293.15;PH=3;Pt = 880;Kl= 0.1;B = 0.33;xin = 0;yin =
0.064
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
```

```
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on,plot(f,u,'k',f,s,'r')
xlabel('The cell number'), ylabel('x/xin, y/yin'),title('The effect of the length of the mixer')
end
end
if i==5
for L=[0.005 0.0167 0.033 0.0667 ];
Kl=0.1;N = 39;V =0.0054;G = 0.00667;T = 293.15;PH=3;Pt = 880;B = 0.33;xin = 0;yin =
0.064;
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on,plot(f,u,'k',f,s,'r')
xlabel('the mixer length, z'), ylabel('x/xin, y/yin'),title('The effect of liquid flow rate')
end
end
if i==6
for T=[293.15  300 310]
 N = 39;V =0.0054;L = 0.03;G = 0.00667;PH=3;Pt = 880;Kl= 0.1;B = 0.33;xin = 0;yin =
0.064
Kd = 5.43*10^3 * exp(-4964/T);H = (3.84*10^7)*((10^(PH-14))^0.035) * exp(-2428/T);
m = H/Pt;a0 = 1+B; a1 = 1+(2*B)+((Kl+Kd)*(V/L)); a2 = B; a3 =(Kl*V)/L; a4 =
(Kl*V)/G;
LM = zeros(N,N);LM = LM + diag(-a1*ones(N,1),0)+ diag(a2*ones(N-1,1),1) +
diag(a0*ones(N-1,1),-1);
LM(1,1)= a2-a1; LM(N,N)= a2-a1;LB = zeros(N,1);LB(1,1)= -xin;
GM = zeros(N,N);GM = GM + diag(-1*ones(N,1),0) + diag(1*ones(N-1,1),-1);GB =
zeros(N,1);GB(1,1)=(-yin);
C = GB -(a4*inv(LM)*LB);A = GM -((a3*a4/m)*inv(LM))-((a4/m)*eye(N,N));
y = inv(A)* C;x = (inv(LM)*LB)-((a3/m)*inv(LM)*inv(A)*C);
xs =(1/m)*inv(A)*C;u = y/yin;xsin = yin/m;s = x/xsin;
f=1:1:39,figure(i),hold on ,plot(f,u,'k',f,s,'r'),
xlabel('The cell number'), ylabel('x/xin, y/yin'), title('The effect of the Temperature')
end
end
```

دراسة تحليلية لتأثير عوامل التشغيل الرئيسية على معدل نقل كتلة الأوزون في الخلاط الثابت الكينيكي باستخدام نموذج التدفق الرجعي في الحالة المستقرة (BFCM)

الملخص

تم استخدام الخلاط الاستاتيكي الكينيكي (KMS) بعمق في عمليات معالجة المياه والمياه العادمة ، وبشكل أساسي في معالجة المياه بالأكسدة لأغراض الأكسدة والتطهير. نظرًا لضرورة زيادة تركيز الأوزون ، تم تطوير قواطع جديدة تعمل بكفاءة على نسبة منخفضة غازات/سائل *يمكن للخلاط الاستاتيكي الكينيكي تلبية هذه المطالب التي تؤدي إلى زيادة في معدل نقل كتلة الأوزون [1]*. الغرض الرئيسي من هذه الورقة هو استخدام نموذج خلية التدفق الرجعي المستمر في الحالة المستقرة (BFCM) الذي طوره كل من Tizaoui و Zhang[1] لتخمين تغير تركيز الأوزون في المراحل السائلة والغازية على طول الخلاط الاستاتيكي الكينيكي KMS. كذلك تهدف الدراسة أيضا إلى تطوير كود Matlab للتدفق الرجعي المستمر في الحالة المستقرة. علاوة على ذلك ، اهتم هذا البحث تأثير عوامل التشغيل الرئيسية: معامل نقل الكتلة السائلة الحجمية (k_L a) ، وطول الخلاط الساكن Kenics ، ومعدل تدفق الماء (L) ، ومعدل تدفق الغاز (G) ، ونسبة التدفق الرجعي (B) ودرجة الحرارة على تركيز الأوزون في المرحلتين الغازية والسائلة (y/y_{in}) و (x/x_{in}^{*}) على التوالي على طول ارتفاع الخلاط الكينيكي الثابت.

الكلمات المفتاحية : نقل كتلة الأوزون ، نموذج خلية التدفق الرجعي ، الخلاط الاستاتيكي الكينيكي